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Progress has been made in all areas, but it is most significant and ready for application to practical models in the case of the CBL. This has resulted from a clear understanding of the vertical structure and diffusion in the CBL, as demonstrated by laboratory experiments, numerical simulations, and field observations. Understanding of turbulence structure and diffusion in the SBL is less complete and not yet ready for general use in applications. However, some promising new developments include a similarity framework for turbulence structure over ideal terrain and models to predict vertical dispersion in terms of the local structure.

As for model uncertainty, it is recommended that natural variability estimates ultimately become an integral part of air quality predictions. Some general frameworks for these estimates include the meandering plume and Eulerian similarity models, with the former being of more immediate utility. However, further evaluation of these models is necessary before they can be recommended for applications.

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Updating Applied Diffusion Models*

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ABSTRACT

Most diffusion models currently used in air quality applications are substantially out of date with understanding of turbulence and diffusion in the planetary boundary layer. Under a Cooperative Agreement with the Environmental Protection Agency, the American Meteorological Society organized a workshop to help improve the basis of such models, their physics and hopefully their performance. Reviews and recommendations were made on models in three areas: diffusion in the convective boundary layer (CBL), diffusion in the stable boundary layer (SBL), and model uncertainty.

Progress has been made in all areas, but it is most significant and ready for application to practical models in the case of the CBL. This has resulted from a clear understanding of the vertical structure and diffusion in the CBL, as demonstrated by laboratory experiments, numerical simulations, and field observations. All of these investigations have shown the importance of the convective scaling parameters: w_*, the convective velocity scale and z_i, the CBL height. This knowledge and the non-Gaussian nature of vertical diffusion have already been incorporated in some applied models and show much promise. The workshop has made a number of recommendations concerning the use of this information, with perhaps the most important being the use of w_*, z_i directly in expressions for the dispersion parameters (σ_y, σ_z).

Understanding of turbulence structure and diffusion in the SBL is less complete and not yet ready for general use in applications. However, some promising new developments include a similarity framework for turbulence structure over ideal terrain and models to predict vertical dispersion in terms of the local structure. Further development and testing of these models are required, with new data sets—laboratory, numerical, and field—being especially beneficial.

As for model uncertainty, it is recommended that natural variability estimates ultimately become an integral part of air quality predictions. Some general frameworks for these estimates include the meandering plume and Eulerian similarity models, with the former being of more immediate utility. However, further evaluation of these models is necessary before they can be recommended for applications.

1. Introduction

Under a Cooperative Agreement with the Environmental Protection Agency (EPA), the American Meteorological Society (AMS) recently conducted a peer review of ten Gaussian diffusion models for tall stacks (Smith, 1984). Based on that review, one would conclude that the models are 10 to 20 years out of date with contemporary understanding of turbulence and diffusion in the planetary boundary layer (PBL). For example, most of the models contained the same components with the following deficiencies:

1) They applied the Pasquill-Gifford dispersion curves (Gifford, 1961) to stack plumes even though the curves are based on passive tracer releases from a ground-level source. It is well-known that dispersion characteristics are quite different for surface and elevated sources in the PBL (Lamb, 1982; Hunt, 1982).

* June 1985—This paper is an overview of the review and recommendations arising from the AMS/EPA Workshop on Updating Applied Diffusion Models held in Clearwater, Florida, January 24–27, 1984. The workshop participants and contributors to this report were: J. C. Weil, Chairman; R. Berkowicz, Riso National Laboratory, Roskilde, Denmark; N. Bowne, TRC-Environmental Consultants Inc., East Hartford, CT; G. A. Briggs, U.S. EPA, Research Triangle Park, NC; R. Britter, University of Cambridge, Cambridge, England; G. Csanady, Woods Hole Oceanographic Institution, Woods Hole, MA; J. W. Deardorff, Oregon State University, Corvallis, OR; K. L. Demerjian, U.S. EPA, Research Triangle Park, NC; R. Draxler, NOAA, Rockville, MD; P. Durbin, NASA, Cleveland, OH; D. G. Fox, USDA Forest Service, Ft. Collins, CO; S. R. Hanna, ERT Inc., Concord, MA; B. Hicks, NOAA, Oak Ridge, TN; T. Horst, Battelle Pacific Northwest Laboratory, Richland, WA; J. C. R. Hunt, University of Cambridge, Cambridge, England; J. Irwin, U.S. EPA, Research Triangle Park, NC; R. McNider, University of Alabama at Huntsville, Huntsville, AL; P. K. Misra, Ontario Ministry of the Environment, Toronto, Canada; D. J. Netterville, Syncrude Canada Ltd., Edmonton, Canada; B. Sawford, CSIRO Division of Atmospheric Research, Mordialloc, Australia; F. Schiermeier, U.S. EPA, Research Triangle Park, NC; M. E. Smith, Meteorological Evaluation Services Inc., Amityville, NY; I. Sykes, ARAP Inc., Princeton, NJ; J. A. Tikvart, U.S. EPA, Research Triangle Park, NC; A. P. van Ulden, Royal Netherlands Meteorological Institute, de Bilt, The Netherlands; A. Venkatram, ERT Inc., Newbury Park, CA; A. Weber, E. I. Dupont de Nemours Inc., Aiken, SC; D. J. Wilson, University of Alberta, Edmonton, Canada; J. C. Wyngaard, National Center for Atmospheric Research, Boulder, CO.

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pp 1111–1130

2) They adopted the Pasquill-Turner empirical method for estimating stability, an approach which ignores the PBL's vertical structure, both mean and turbulent. Moreover, it is strongly biased toward neutral stability when convective conditions actually exist (e.g., see Weil and Brower, 1984).

3) They used a simple "all or none" technique for predicting buoyant plume penetration of elevated stable layers and neglected the major impediment to penetration—the stratification aloft.

As indicated, these models should not be considered representative of diffusion research over the past two decades; for a summary of the latter see Nieuwstadt and van Dop (1982) or Pasquill and Smith (1983).

In addition to the above deficiencies, the models performed poorly, as judged from a comparison between predicted and observed SO_2 concentrations around the Clifty Creek (Indiana) power plant. However, the "experiment" for testing the models was far from ideal, being based on comparisons at only six ground-level monitors. The sparse monitoring network coupled with insufficient wind data precluded an accurate determination of the transport direction. Furthermore, the comparisons were plagued by other meteorological data limitations and by the "natural" variability in concentrations (Smith, 1984), which arises from the stochastic nature of the flow and is large (order of the mean concentration).

The prediction of dispersion parameters (σ_y, σ_z) directly from turbulence measurements and statistical or other appropriate theory has long been considered the preferred approach (e.g., Pasquill, 1961). Contributions and successful demonstrations of this approach can be found for example in Slade (1968), Draxler (1976), Irwin (1983), and Pasquill and Smith (1983). However, reliable turbulence data are rarely available in regulatory applications, and therefore, one must estimate it. In the past, such estimates have presented one of the main challenges and needs, i.e., a realistic PBL turbulence description in terms of a minimum number of observables (wind speed, insolation, etc.). However, in the last decade or so, substantial progress has occurred in our understanding and prediction of PBL structure and its effect on diffusion. This has been achieved by a collective effort of theoretical and numerical modeling, laboratory simulations, and field observations as summarized, for example, in the Nieuwstadt and van Dop (1982) monograph. It is perhaps most notable for the daytime, convective boundary layer (CBL), but has recently been achieved for the nocturnal, stable boundary layer (SBL); e.g., Wyngaard (1983).

Inspired by the PBL knowledge and the generally poor state of "regulatory" modeling, the AMS Steering Committee for the EPA Cooperative Agreement organized a workshop to help close the wide gap between the two. The focus was on diffusion from a point source at arbitrary height in the PBL and over distances less than ~20 km; interest was generally in one-hour averaged concentrations. The workshop purposes were to review current PBL understanding and its use in diffusion models not included in the Smith review and to recommend improved ones; i.e., models with better physics and hopefully better performance than those summarized by Smith (1984).

The workshop was divided into a day and a half session of review papers and two days of subgroup discussions. The papers were: 1) "Structure of the planetary boundary layer and implications for its modeling" by J. C. Wyngaard, 2) "Laboratory experiments on diffusion: the use of convective mixed-layer scaling" by J. W. Deardorff, 3) "A review of Lagrangian statistical simulations of concentration mean and fluctuation fields" by B. L. Sawford, 4) "Analytical parameterizations of diffusion: the CBL" by G. A. Briggs, 5) "Diffusion in the stably stratified atmospheric boundary layer" by J. C. R. Hunt, 6) "Estimation of atmospheric boundary layer parameters for diffusion applications" by A. P. van Ulden and A. A. M. Holtslag, and 7) "Diffusion applications including buoyant sources" by J. C. Weil. The written manuscripts of the first six papers appear in this edition of the *Journal of Climate and Applied Meteorology*.

Three subgroups were formed to discuss and make recommendations on: 1) diffusion in the CBL, 2) diffusion in the SBL, and 3) model uncertainty; they were chaired by J. Irwin, A. van Ulden, and D. J. Wilson, respectively. The first two topics dealt with models for the mean concentration field and all related aspects—PBL structure, applied model approaches, etc. The separate discussion of the CBL and SBL was motivated by their very different character and by the difference in our understanding of them; knowledge of the CBL is much further advanced. Model uncertainty focused on the determination of the "natural" variability in the concentrations. It is necessary to know this for both model verification and for predicting exceedances of specified concentration levels, i.e., air quality standards.

In the following, we briefly summarize the status of the three topics, note some of the important unsolved problems, and give our recommendations. The recommendations on models for the CBL are more specific and of more immediate use because of our better understanding of it. For the SBL and model uncertainty, further model development and testing are needed to put new information into practice. The participants in this workshop are responsible for the substance of this report.

2. Diffusion in the convective boundary layer

In this section, we review the main features of turbulence structure and diffusion in the CBL, describe applied diffusion models incorporating some of them, and then give our recommendations.

a. CBL structure

The CBL extends from the ground to the base of an elevated stable layer and is characterized by strong vertical mixing driven by upward heat flux. Deardorff's (1972) numerical simulations first revealed the detailed structure of the layer and showed that the most important turbulence length and velocity scales were z_i, the CBL depth, and w_*, the convective velocity scale; $w_* = (gQ_0 z_i/\rho c_p T)^{1/3}$, where g is the gravitational acceleration, Q_0 the surface heat flux, and ρ, T, and c_p are the air density, temperature, and specific heat at constant pressure. The success of z_i and w_* in ordering turbulence data has been demonstrated over a broad range of scales: from laboratory experiments (Willis and Deardorff, 1974) to full-scale field observations (Kaimal *et al.*, 1976; Caughey, 1982). At midday, typical values of z_i and w_* are 1 to 2 km and 2 m s^{-1}, respectively.

Turbulence arising from wind shear is generally confined to small heights, $z < -L$, where L is the Monin-Obukhov length. $L = -\rho c_p T u_*^3/kgQ_0$ where u_* is the friction velocity and k the von Karman constant ($\sim$0.4). In the bulk of the CBL, the stability parameter measuring the relative effects of convection and wind shear is $z_i/-L$, which can be expressed alternatively by w_*/u_*. If one assumes a typical resistance coefficient, u_*/u (say 0.05) where u is the mean wind speed, then u can replace u_* (Deardorff and Willis, 1974), but retention of u_* is preferred in general because it accounts for the local roughness. At midday, $z_i/-L$ is usually large (>10), indicating the dominance of convective turbulence throughout the bulk of the CBL.

For simplicity, the CBL can be considered to be horizontally homogeneous and to have a vertical structure comprising three layers: surface, mixed, and entrainment interfacial. In the surface layer ($z < 0.1z_i$), the mean wind and potential temperature exhibit strong gradients. The crosswind turbulence component, σ_v, is independent of height, but depends on u_* and $z_i/-L$ according to an interpolation formula (Panofsky *et al.*, 1977):

$$\sigma_v/u_* = [4 + 0.6(z_i/-L)^{2/3}]^{1/2}; \quad (1)$$

the vertical component, σ_w, is found to follow a similar expression but with different constants and z_i replaced by z. In the mixed layer ($0.1z_i < z < 0.8z_i$), the mean wind, potential temperature, and the turbulence components show relatively little height variation; σ_v, $\sigma_w \sim 0.6w_*$. In the interfacial layer ($0.8z_i < z < 1.2z_i$), all variables gradually approach their values above the CBL.

The convection elements in the CBL consist of thermal plumes or updrafts surrounded by large downdrafts; both extend from near the surface into the interfacial layer. For sufficiently unstable conditions, the elements are randomly distributed and long-lived, having time scales z_i/w_* of $\sim$10 min. Hunt (1984) discusses how the turbulence structure can be analyzed quantitatively in terms of eddies impinging on the ground and the elevated inversion base.

b. Diffusion characteristics

Our understanding of passive tracer diffusion in the CBL was significantly advanced by the laboratory experiments of Willis and Deardorff (1976, 1978, 1981) and the numerical simulations of Lamb (1979, 1982). Their investigations clearly showed the effect of source height, h_s, on the diffusion patterns and the utility of convective scaling (w_*, z_i). For elevated sources ($h_s > 0.1z_i$), the average plume centerline, as defined by the locus of mean maximum concentration, descended within a short distance from the source until it reached the ground. The descent was explained by the organized, long-lived thermal motion in the CBL and by the fact that downdrafts occupied a greater fraction (0.6) of the horizontal surface area than did updrafts. The behavior was recently confirmed in a field experiment at the Boulder Atmospheric Observatory (Moninger *et al.*, 1983).

In contrast, the average centerline from near surface releases ($h_s < 0.1z_i$) ascended after a short downwind distance. This behavior resulted from the "sweep out" of material near the surface before material initially carried aloft recirculated down. The behavior for both source types differs strongly from that assumed in the Gaussian plume model.

The laboratory experiments demonstrated another important aspect of diffusion: a turbulent flux opposed to the local concentration gradient in certain regions (Deardorff and Willis, 1975). Similar findings have been obtained by Wyngaard and Brost (1984) and Moeng and Wyngaard (1984) based on large eddy simulations. These results put the applicability of eddy diffusivity (K) approaches on very tenuous ground since negative K values and singularities occur.

The dispersion parameters found in the laboratory and numerical simulations were in excellent agreement with one another when suitably nondimensionalized (e.g., Lamb, 1982). The σ_y/z_i and σ_z/z_i were shown as functions of a nondimensional distance, X:

$$X = w_* x/uz_i, \quad (2)$$

which is the ratio of travel time, x/u where x is the downwind distance, to the turbulence time scale z_i/w_*. For the elevated releases, the dispersion parameters were linearly dependent on X at short range ($X < 1$), consistent with the short-range limit of statistical theory; this was attributed to the quasi-homogeneity of turbulence in the upper part of the CBL. For the near surface sources, the short range σ_z increased as $X^{6/5}$ (Lamb, 1979), in qualitative agreement with Yaglom's (1972) surface layer similarity theory ($\sigma_z/z_i \propto X^{3/2}$); this was due to the increase of σ_w with height in the surface layer. In addition, these results were generally consistent with the field observations summarized by Briggs (1985a) and Nieuwstadt (1980).

More recently, Willis and Deardorff (1983) simulated the rise and dispersion of buoyant plumes in their convection tank. The simulations showed that the most important dimensionless measure of plume buoyancy in the far field was $F_* = F/uw_*^2 z_i$, where F is the stack buoyancy flux (proportional to the heat flux). For $F_* < 0.03$, the plume behaved somewhat like that from a nonbuoyant source after some initial rise. However, for $F_* \sim 0.1$, the plume rose to the top of the CBL, partially penetrated into the entrainment interfacial layer, and only gradually mixed downward in the CBL. The latter behavior suggested that the two part Gaussian model—plume rise followed by dispersion about an effective stack height (i.e., a single point source)—is not appropriate.

Subsequent measurements (Willis and Hukari, 1984) have more clearly demonstrated the highly skewed nature of the vertical concentration distribution. Moreover, these measurements as well as those by Deardorff and Willis (1984) showed the substantial reduction in ground-level concentrations due to plume buoyancy.

Modeling of the far-field buoyancy effects has addressed two key problems: "final rise" due to ambient turbulence and plume penetration of elevated inversions. In view of the Willis and Deardorff results, the concept of final rise (due to turbulence) may only be relevant for the smaller F_* range above.

Briggs (1975, 1984a) proposed two final rise models that incorporate some of the more contemporary CBL physics. The first assumes that plume "break-up" and final rise occur when the turbulence dissipation rate inside the plume decays to that in the surrounding environment. In strong convection, the prediction is:

$$\Delta h = 3F_*^{3/5} z_i. \tag{3}$$

In weak convection and strong winds (large L), the rise prediction for a neutral boundary layer can be assumed. It is

$$\Delta h = 1.2F_n^{3/5}(1 + 1.2F_n)^{2/5} h_s, \tag{4}$$

where $F_n = F/uu_*^2 h_s$. Equation (4) is an approximation (Briggs, 1984b) to the final rise formula in Briggs (1975, 1984a); it matches the small and large F_n limits of the latter and avoids iterative solution. The second model, "touchdown," describes the effect of large scale meandering on the plume. It assumes that a plume is brought to ground by the downdrafts in the CBL and predicts the "effective rise" in terms of the mean downdraft velocity, u, z_i, and h_s. Due to the lack of "final rise" observations, little direct testing of these models has occurred although some support is given in Weil (1979) and Briggs (1975).

Plume penetration models exist for two cases of stability capping the CBL: a thin inversion characterized by the potential temperature jump at z_i, and a thick inversion characterized by the potential temperature gradient, $\partial\theta_a/\partial z$, in the elevated layer. For the first case, models by Briggs (1984a) and Manins (1979) predict penetration based on the same nondimensional parameter, but differ strongly on the degree of penetration, the former predicting much more. This controversy needs resolution with further analytical and laboratory modeling. For a thick inversion, Briggs (1984a) conservatively estimated penetration assuming that the stable layer lapse rate extended from the inversion down to the stack top; the model was supported by some field observations. Berkowicz *et al.* (1985) made a slight extension to the model by assuming that the plume would not feel the elevated inversion until its upper edge reached the inversion base. Their prediction for the effective rise, from which the degree of penetration is determined, is:

$$\frac{\Delta h}{z_i'} = \left[2.6^3\left(\frac{F}{uN_a^2 z_i'^3}\right) + (2/3)^3\right]^{1/3}, \tag{5}$$

where $z_i' = z_i - h_s$ and $N_a = [(g/T_a)(\partial\theta_a/\partial z)]^{1/2}$.

c. *Applied models*

In the following, we discuss alternative models for estimating diffusion in the CBL, general functional forms for the dispersion parameters (σ_y, σ_z) when Gaussian profiles are assumed, and methods for estimating key CBL variables needed in the models.

1) DIFFUSION

There are essentially three types of applied models in which improved CBL understanding has been incorporated: 1) the Gaussian model, 2) the probability density function (pdf) approach, and 3) the "impingement" model. All models assume Gaussian profiles in the lateral direction; the Gaussian model also adopts this profile in the vertical.

In the Gaussian category, Weil and Brower (1984) and Berkowicz *et al.* (1985) included model components based on some of the previously discussed information. They chose Briggs' (1975) plume rise models, Briggs' (1984a) criteria (or modified) for plume penetration of inversions, and dispersion parameters incorporating u/w_* or $z_i/-L$ as the measure of stability. Weil and Brower adopted Briggs' dispersion curves, which were intended for elevated releases and are generally consistent with statistical theory, at least for short range (i.e., $\sigma_y = \sigma_v x/u$). Using interpolation formulas for the turbulence components similar to Eq. (1), they related the curves directly to u/w_*. Evaluation of their model with ground-level SO_2 concentrations downwind of several Maryland power plants showed that it performed much better than the EPA CRSTER model. However, a later evaluation by EPA (Tikvart and Cox, 1984) indicated that the model overestimated the maximum SO_2 concentrations around the Clifty Creek power plant by factors of ~2–3. The maximum concentrations were predicted to occur under low z_i (~500 m) when the plume was not predicted to penetrate the

elevated inversion. Improved modeling of this situation is a high priority task.

While improved Gaussian modeling can lead to better performance, we must remember this model's limitations. First, real plumes are not Gaussian in the vertical as demonstrated by the laboratory and numerical simulations discussed earlier. Thus, improved σ_z and plume rise expressions can only result in approximate matching of the axial ground-level concentration distribution. Second, the model is an inadequate description of dispersion under conditions of plume penetration of inversions, with potential reentrainment, or when strongly buoyant plumes loft at the CBL top; these problems require much more attention.

One of the deficiencies of the Gaussian model—the vertical distribution—can be overcome by the pdf model. In the latter, the concentration field is computed from the pdf of vertical velocity under the assumption of infinitely long turbulence time scales. Models developed by Misra (1982), Venkatram (1983), and Weil and Furth (1981) included a skewed pdf (i.e., non-Gaussian) based on the earlier cited laboratory and numerical simulations and on Lamb's (1982) numerical results. The models produced qualitative and, in some cases, good quantitative agreement with the laboratory and numerical simulations. However, extensions are necessary to treat buoyant sources and to deal with dispersion in the neutral limit ($z_i/-L < 1$), where the assumed pdf may be inappropriate.

A third applied approach is the impingement model for buoyant sources (Venkatram, 1980a). In this model, the ground-level concentration distribution is found from an assumed pdf of the impingement distance, the point where plume segments caught in downdrafts first touch the ground. The mean impingement distance is found from Briggs (1975) touchdown model for plume rise. Evaluation of this model around several large point sources shows very good performance. The model needs generalization to account for zero or weakly buoyant sources and the neutral stability limit.

The three models discussed above are restricted to steady state and neglect axial diffusion; the latter is important when $u/w_* \leqslant 1.2$ (Willis and Deardorff, 1976). One approach that can treat these problems is the puff model (e.g., Csanady, 1973), but it has generally not seen much use in applications. However, we feel that it should because current practice for treating "calm" conditions is to apply the Gaussian model with an arbitrarily small wind speed ($\sim$1 m s^{-1}). This approach may lead to unrealistically high concentrations, especially when z_i is small and no inversion penetration occurs.

It should be emphasized that these models and the discussion in the previous two sections apply to a horizontally homogeneous CBL. There is increased awareness that any local heat flux perturbations (rivers, lakes), which affect the mean circulation, also can have noticeable effects on diffusion. This should be remembered in model applications and evaluations, especially since many sources (e.g., power plants) are located near lakes or rivers.

2) Dispersion parameters

General expressions are desired for σ_y, σ_z that satisfy the appropriate time dependence and reduce to the correct limits in fully convective or neutral conditions. For σ_y, there is general agreement that a suitable form is (Pasquill, 1971, Hanna *et al.*, 1977):

$$\sigma_y = \sigma_v t f(t/\tau_{Ly}) \tag{7}$$

where t is time and τ_{Ly} is the Lagrangian time scale; t can be replaced by x/u when axial diffusion is unimportant. A useful function that matches the short and long time limits of statistical theory is:

$$f(t/\tau_{Ly}) = \frac{1}{(1 + t/2\tau_{Ly})^{1/2}} \tag{8}$$

(e.g., Deardorff and Willis, 1975).

In strong convection ($z_i/-L > 10$) with $\tau_{Ly} \propto z_i/w_*$, $\sigma_v = 0.6w_*$, and $t = x/u$, the nondimensional σ_y given by Eqs. (7) and (8) is

$$\frac{\sigma_y}{z_i} = \frac{0.6X}{(1 + \alpha X)^{1/2}}, \tag{9}$$

where α depends on the proportionality coefficient between τ_{Ly} and z_i/w_*; its value is somewhat uncertain. Field observations (Briggs, 1985a; Weil, 1983) suggest α to range from 0 to $\sim$2, with a typical value of $\sim$0.7 (inferred $\tau_{Ly} = 0.7z_i/w_*$). Deardorff and Willis' laboratory data yield $\alpha = 0.91$, with $\tau_{Ly} = 0.55z_i/w_*$. The variability in the field data is partially associated with the large and variable time scale of mesoscale eddies; this problem merits much further attention. Whatever the choice for α, Eq. (9) is suitable for surface as well as elevated sources in the CBL because of the small height dependence of σ_v and u.

For weaker convection ($0 < z_i/-L < 10$), σ_v can be determined from an interpolation formula like Eq. (1). However, there is no consensus on a general formulation for τ_{Ly}. Possibilities are: $\tau_{Ly} \propto z_i/\sigma_v$ (Smith and Blackall, 1979); $\tau_{Ly} \propto \sigma_v^2/\epsilon$ (Baerentsen and Berkowicz, 1984), where ϵ is the turbulent energy dissipation rate (parameterized in terms of w_*, u_*, z, and z_i); or $\tau_{Ly} \propto f_1(-h/L)h/u_*$, where $h = z_i$, in the convective limit and $h = 0.3u_*/f$ in the neutral limit, f being the Coriolis parameter (Nieuwstadt and van Duren, 1979). At this point, a choice of these possibilities is a matter of taste. Further investigation is necessary with field data in the near-neutral limit being especially helpful.

For σ_z, one must consider source height dependence because of the variation of σ_w with z. In strong convection and for $z > 0.1z_i$, such variation is small; $\sigma_w \sim 0.6w_*$. Statistical theory predicts $\sigma_z/z_i = 0.6X$, which is in close agreement with the earlier cited laboratory and numerical simulations. Beyond $X \sim 0.7$, the sim-

ulations show $\sigma_z \sim$ constant, due to plume trapping in the CBL. In the Gaussian model, this is simulated by plume reflection at $z = z_i$.

In less unstable conditions, particularly as $z_i/-L \to 0$, σ_z may tend towards a $t^{1/2}$ dependence at long times due to the shorter time scales in the neutral limit. Such a dependence could arise before plume trapping occurs, i.e., before a uniform vertical distribution is attained. Thus, a tentative general form for σ_z is similar to that for σ_y [Eqs. (7) and (8)], and requires the parameterization of τ_{Lz}.

For surface sources ($h_s < 0.1z_i$), Deardorff and Willis (1975) suggested an interpolation formula for the short range ($\sigma_z/X < 0.5$), based on their laboratory data. It matches the neutral and free convection limits and is

$$\frac{\sigma_z}{z_i} = \left[\left(\beta \frac{u_*}{w_*} X\right)^2 + 0.25X^3 + 1.8h_s^{*2/3}X^2\right]^{1/2}, \quad (10)$$

where

$$\beta = \frac{0.4 + 0.8(w_*h_s^*/u_*X)}{1 + (w_*h_s^*/u_*X)} \quad (11)$$

and $h_s^* = h_s/z_i$; Briggs (1985b) suggests multiplying β by 1.6 to provide better agreement with field data. Use of Eq. (10) in the Gaussian model should approximate ground-level concentrations for $X < 0.5$ and is expected to overestimate them somewhat beyond that range.

3) CBL VARIABLES

The diffusion models require measurements or estimates of key boundary layer variables—Q_0, u_*, $u(z)$, and z_i, from which others can be determined, e.g., w_* and L. Generally, the key variables are not routinely measured and must therefore be estimated from available data. As a minimum, it is assumed that the following are available: wind and temperature measurements from a 10-m tower, cloud cover observations, and early morning temperature profiles over the lowest ~2 km of the PBL.

Holtslag and van Ulden (1983) show that Q_0 and u_* can be estimated from routine data. Based on the surface energy budget, the Q_0 is assumed proportional to the net radiation, which can either be measured or estimated (from the insolation, computed longwave radiation, and the albedo). The u_* is determined from a wind measurement at a single height using the similarity wind profile:

$$u = (u_*/k)[\ln(z/z_0) - \psi(z/L)], \quad (12)$$

where z_0 is the roughness length and ψ is a stability correction function. The z_0 can be determined from visual inspection of the site (e.g., Wieringa, 1980) or deduced from the similarity profile if wind measurements are available at multiple heights (Nieuwstadt, 1978). The Holtslag and van Ulden scheme has been successfully demonstrated over a simple grass-covered surface; however, it includes parameters that can be adjusted to other surfaces but remains to be tested against them.

In the preceding Q_0 approach, an empirical, site-dependent parameter must be specified to characterize the surface moisture. Alternative methods are available. One (Berkowicz and Prahm, 1982) depends on a humidity measurement to indicate the evaporation potential, the integrated net radiation since the last rainfall, and several empirical constants. A second is the profile method but with wind speed and temperature available at multiple heights on a tower (e.g., Irwin and Binkowski, 1981; Nieuwstadt, 1978). In strong convection, one could use Dyer's (1965) method, which depends on the potential temperature difference between two heights. In general, the characterization of surface moisture is the most significant problem in predicting Q_0.

In strongly convective conditions ($z_i/-L > 10$), the wind profile follows the similarity relation up to $0.1z_i$ and is essentially flat above the latter (Garratt *et al.*, 1982). For $z > 0.1z_i$, the wind speed is given by the similarity expression evaluated at $0.1z_i$. In weaker convection, $u(z)$ is given approximately by the similarity expression throughout the CBL.

The CBL height can be predicted from simple energy balance or slab models (e.g., Carson, 1973; Driedonks, 1982; Tennekes, 1973). They require an early morning temperature profile and the timewise integrated surface heat flux.

d. Recommendations for applied models

As a result of this review, the following recommendations are made.

1) *Model approach*—For the short term, the Gaussian model is recommended principally because of its present capability to deal with buoyant sources and with dispersion over a continuous range of stability; however, its limitations should be remembered. For the longer term, the pdf model may be a better approach, especially in dealing with non-Gaussian vertical structure. We encourage its extension to treat buoyant plumes and the neutral stability limit. The impingement model is another approach with demonstrated success, but which needs modification to handle neutral stability and weakly buoyant plumes. For all models, an important problem to be dealt with is dispersion during partial plume penetration of inversions and/or plume lofting at the CBL top.

2) *Plume rise and buoyancy effects*—The Briggs (1975, 1984a) formulas discussed earlier are recommended for estimating final rise. In practice, the lowest estimate from the alternative formulas should be used. This is an interim recommendation as the concept of "final rise" in convective conditions is somewhat uncertain. For plume penetration of inversions, a tentative recommendation is to use the Berkowicz *et al.* (1985)

modification of Briggs' model for estimating the effective plume height (Eq. 5), which is then used to determine the plume penetration factor (see Briggs, 1984a). Further work is necessary to determine the theoretical and practical merits of this approach, applicable for thick, elevated stable layers, versus the thin inversion model (e.g., Manins, 1979).

3) *Dispersion parameters*—Our key recommendation is that convective scaling (w_*, z_i) should be used in the strongly convective limit with σ_y given by Eq. (9) and σ_z by $\sim 0.6 w_* x/z_i$. For arbitrary stability, interpolation formulas of the type discussed under section 3c2 should be used for estimating σ_y, σ_z; i.e., formulas that approach the appropriate time dependence (t or $t^{1/2}$) and stability limits (strongly convective or neutral). The expressions discussed here meet the spirit of this recommendation, but others are possible. The turbulence components (σ_v, σ_w) can be estimated from expressions like Eq. (1) (see also Weil and Brower, 1984; Berkowicz *et al.*, 1985; Briggs, 1985b). Alternatively, direct measurements of σ_v, σ_w can be used provided that they are properly averaged over the layer in which diffusion occurs or extrapolated to it. (In the case of σ_w, one must consider its vertical profile.)

4) *CBL parameters*—For simplicity, the Holtslag and van Ulden (1983) approach is recommended for estimating Q_0 and u_*. For Q_0, alternative methods could be used provided that additional measurements are available (relative humidity and integrated net radiation since last rainfall or wind speed and temperature at multiple heights). The similarity profile and a simple adaptation (as discussed under section 3c3) are recommended for estimating the wind, and a slab or energy balance model for z_i.

5) *Model evaluation*—In the development and evaluation of models, we strongly urge that one uses all relevant data including the numerical (Lamb) and laboratory simulations (Deardorff and Willis) discussed earlier. These simulations are especially helpful because of their conduct during controlled external conditions (u, Q_0, z_i). Additional numerical simulations with large eddy models would be of much benefit in enhancing this data base (see Wyngaard *et al.*, 1984). Furthermore, we encourage use of field data sets with as complete a description of the concentration field as possible (dense sampling networks, remote sensing of elevated plumes, etc.) and of the meteorological input—Q_0, $u(z)$, z_i, turbulence, etc. The Electric Power Research Institute's experiments at the Kincaid power plant are one example (e.g., Bowne *et al.*, 1983). However, in using field data, one must be cognizant of any local roughness or heat flux perturbations (e.g., large rivers or lakes), which may lead to measurable departures in dispersion relative to the ideal, homogeneous terrain case.

6) *Key problems*—At present, the main problems in applied diffusion modeling are viewed to be associated with source buoyancy effects. These include: 1) the prediction of diffusion during partial plume penetration of inversions; 2) the lofting/slow downward diffusion of strongly buoyant, nonpenetrating plumes from the CBL top; and 3) the prediction of "final rise." Briggs (1985b) gives a preliminary approach for dealing with lofting, strongly buoyant plumes. Other important problems are the estimation of diffusion during light or zero winds and prediction of the Lagrangian time scales from routine data. The problem for τ_{Ly} exists for all stabilities, but for τ_{Lz} it is restricted primarily to the neutral limit.

3. Diffusion in the stable boundary layer

The format of this section follows that for the CBL. In order, we discuss: SBL structure, diffusion characteristics, applied models, and our recommendations.

a. SBL structure

In contrast to the CBL, turbulence in the SBL is driven by shear stress, and is inherently much weaker than in the CBL. The stress, which has a maximum at the surface, decreases monotonically with height to near zero at the SBL top. The turbulence velocity scale is u_*, which is typically 0.1 to 0.3 m s^{-1}, while the SBL height ranges from a few meters to a few 100 m. In general, we know less about turbulence in the SBL than in the CBL due to the greater measurement problems (smaller turbulence levels) and to the complications arising from gravity waves and local drainage effects (Wyngaard, 1983). Furthermore, the SBL is not stationary but evolves slowly with time in response to changing surface conditions (typical time scale of ~3–10 hours; see Brost and Wyngaard, 1978).

Given these complications, a universal picture of the turbulence structure does not exist for all SBLs. However, it does exist (Nieuwstadt, 1984a) for an idealized, continuously turbulent SBL in which waves, drainage flows, and intermittency can be ignored. Such a boundary layer can exist over very flat terrain in the presence of moderate to strong geostrophic winds (≥5 m s^{-1}), where the stability would be characterized as weak to moderately stable.

Nieuwstadt's description is based on the solution of a set of turbulence closure equations used in a second order model (Brost and Wyngaard, 1978) under the assumption of local scaling. Turbulence profiles are obtained by coupling the turbulence closure to rate equations for the mean wind and temperature, but simple solutions are found only for the case of a stationary SBL. For the latter, the profiles reduce to similarity expressions. The form for σ_w is

$$\sigma_w/u_* = 1.4(1 - z/h)^{3/4}, \qquad (13)$$

where $h \propto (u_* L/f)^{1/2}$, as given earlier by Zilitinkevich (1972). Nieuwstadt shows that, with the exception of temperature fluctuations, the predicted profiles are in good agreement with turbulence measurements from

a 213-m tower at Cabauw, The Netherlands. (It should be noted that observations with strong gravity wave effects were removed from the analysis.)

One important feature of the SBL is its strong vertical inhomogeneity as demonstrated by the turbulence profiles (Nieuwstadt, 1984a; Hunt *et al.*, 1983; Caughey *et al.*, 1979). Inhomogeneity is also exhibited in the mean wind and temperature (Caughey *et al.*, 1979) and in the turbulence length scale. The latter is proportional to z near the surface but to σ_w/N at large heights (Brost and Wyngaard, 1978), where N is the Brunt-Väisälä frequency; the limiting value—σ_w/N, typically ~ 10 m—is due to the suppression of vertical motion by the stable buoyancy forces.

Nieuwstadt's success in describing turbulence profiles throughout the SBL at Cabauw is certainly encouraging. But it cannot be guaranteed for other sites where terrain inhomogeneities and/or wave effects are present (see Hunt *et al.*, 1983); nor can it be guaranteed when the above effects are absent, but time evolution of the boundary layer is more pronounced. In the nonstationary case, one expects that the turbulence profiles may have a universal shape, but that h will change with time. The time dependence can be computed from a rate equation given by Nieuwstadt and Tennekes (1981). The equation is based on an analysis of the turbulence kinetic energy budget and has the form

$$\frac{dh}{dt} = \frac{h_{ss} - h}{T} \tag{14}$$

where h_{ss} is the steady state solution [$\propto (u_* L/f)^{1/2}$] and T is a relaxation time scale. At present, the main difficulty in applying this equation lies in estimating the initial SBL height, i.e., at evening transition.

Another potentially important behavior can occur during extreme stability when rather quiescent flow over a relatively long period is interrupted by "bursts" of turbulence throughout the entire SBL (Schubert and Pepper, 1976). The cause of this behavior is not well defined, but waves and shear instabilities are possibilities.

In summary, the similarity model is a useful departure point for estimating SBL turbulence structure over ideal (flat) terrain, unencumbered by wave effects, strong nonstationarity, etc. Further measurements and analysis are required at other sites under varying terrain conditions to: establish the model's limits; further assess wave, drainage, and intermittency effects; and test the rate equation model for h. As a result of these analyses, one can then develop more general engineering correlations for mean and turbulence profiles that can be used in diffusion applications.

b. *Diffusion characteristics*

1) VERTICAL DIFFUSION

The vertical inhomogeneity of mean flow and turbulence in the SBL preclude the writing down of a general expression for the concentration field for a source at arbitrary height. The degree to which inhomogeneities are important depends on source height. Thus, it is helpful to summarize diffusion theories and observations in terms of the source height relative to the vertical structure. We consider in order: surface sources, elevated sources within the surface layer ($h_s < L$), and elevated sources above the surface layer ($L < h_s < h$). Another category is $h_s > h$, but ground-level concentrations resulting from such sources should generally be quite small.

Theory and experiment are most complete for sources within the surface layer. For ground releases, similarity and K theories can successfully predict the vertical spread of a plume at short range in terms of the basic boundary layer variables—u_*, L, and z_0. Gifford (1962), Horst (1979), and Chaudry and Meroney (1973a) demonstrated this for the similarity approach, finding good agreement between their predictions and field observations; additional confirming data were obtained in a stratified wind tunnel (Chaudry and Meroney, 1973b). Using K theory, Nieuwstadt and van Ulden (1978) numerically solved the diffusion equation with wind and diffusivity profiles specified by the Monin-Obukhov expressions. They also found good agreement between their predictions and field measurements. As a result of these analyses, we have a reasonably good understanding of short-range diffusion from a surface source.

For elevated sources in the surface layer, K theory can be strictly used only when $t > \tau_L$ (Hunt, 1982). However, Csanady (1973) described a simple modified method using a transformed distance variable that asymptotically matches both the short ($t < \tau_L$) and long time limits for a point source plume. In principle, the advantage of this method or K theory, in general, is in accounting for the vertical variation in the turbulence and wind shear. One main effect of shear is in depressing the height of the maximum concentration. This phenomena has been predicted (Csanady, 1973; Hunt, 1982) and observed, both in the field (Doran *et al.*, 1978) as well as in wind tunnel experiments (Davar and Cermak, 1964). Its overall effect on ground-level concentrations remains unclear.

In principle, statistical theory cannot legitimately be used in the surface layer because of the inhomogeneity in the mean wind and turbulence. However, out of necessity, it often is used in applications as discussed later. One issue to be resolved is the use of an image plume to handle the "no-flux" surface condition. If the plume reaches the surface via transport by small eddies ($t > \tau_L$), then reflection and image plumes make sense. But if the plume is brought to ground by "large" impinging eddies ($t < \tau_L$), the surface concentration may be more nearly equal to that in these eddies as in flow near a stagnation point, i.e., without the reflection term. Wind tunnel simulations and numerical calculations would help resolve this issue.

For sources above the surface layer, dispersion is controlled for a long distance downwind by turbulence and mean flow at the source height. This is due to the small eddy size ($\sim\sigma_w/N$) and the low turbulence intensity ($\sim$0.03). Then it is useful to quantify the vertical diffusion in terms of the local mean wind and turbulence. Two models do this in light of the key variables, σ_w and N: one by Venkatram *et al.* (1984) and another by Pearson *et al.* (1983), based on an extension of an earlier theory by Csanady (1964).

By ignoring vertical inhomogeneity in the turbulence and mean flow, Venkatram *et al.* assume that statistical theory can describe the vertical dispersion. They adopt a functional form that matches the short and long time limits of the theory (same as Eqs. 7 and 8):

$$\sigma_z = \frac{\sigma_w t}{(1 + t/2\tau_{Lz})^{1/2}}. \tag{15}$$

A key point of their model is that the Lagrangian time scale (τ_{Lz}) is assumed to be l/σ_w, where l is the turbulence length scale and is given by the interpolation formula: $l^{-1} \approx l_n^{-1} + l_s^{-1}$. Here, l_n and l_s denote the scales in the small and large height limits: $l_n = \lambda h_s$, and $l_s = \gamma^2\sigma_w/N$, where $\lambda = 0.36$ and $\gamma = 0.52$. This form for l is the same proposed by Brost and Wyngaard (1978). (An earlier model by Draxler (1976) gives a functional form similar to Eq. 15, but it adopts a constant time scale.)

Venkatram *et al.* found that their σ_z predictions agreed well with field observations of an elevated, neutrally buoyant plume in the SBL; the plume observations extended to $x \sim 1$ km. However, at large times ($tN > 1$), the scatter is sufficient that the data actually lie between lines $\sigma_z \propto$ constant and $\sigma_z \propto t^{1/2}$. The σ_w and N in the experiments were obtained from measurements near the release height, which was typically 50 m; no measurements were made of the SBL height.

The theory developed by Pearson *et al.* (1983) and Csanady (1964) recognizes that molecular mixing between fluid elements must occur if vertical diffusion is to extend over a scale greater than σ_w/N. It is a random force model based on the Langevin equation. For short times, $t \ll N^{-1}$, the predicted σ_z is the same as given by statistical theory: $\sigma_z = \sigma_w t$. For long times, the prediction can be expressed as

$$\sigma_z = (\sigma_w/N)(\zeta_z^2 + 2N^2 t\tau_{Lz})^{1/2} \tag{16}$$

where $\tau_{Lz} = \gamma^2 N^{-1}$; ζ_z is a dimensionless parameter ($\sim$1.2) dependent on the turbulence spectrum; and γ is a dimensionless parameter measuring the degree of mixing between fluid elements. The expected range of γ is 0.1 to 0.4 (Hunt *et al.*, 1983); methods for estimating γ and ζ_z are discussed by Hunt (1982, 1985).

Given the above γ, two limiting cases of σ_z at long times can be observed. If $\gamma \approx 0.1$, the plume thickness approaches a constant, $\sim\sigma_w/N$, over a considerable range of time. But if $\gamma \sim 0.3$, the σ_z approaches a parabolic growth ($t^{1/2}$), consistent with statistical theory and the Venkatram *et al.* model. Pearson *et al.* (1983) cited a few examples of plume measurements that showed both types of behavior. However, measurements of the SBL depth and independent determinations of γ were not available.

The SBL group recognized that plume behavior between the limiting cases of constant σ_z and σ_z growing as $t^{1/2}$ has been observed for an elevated plume. Detailed field, laboratory, and computer simulations paralleling those discussed for the CBL are needed to help resolve the circumstances under which each should occur.

One well-understood aspect of diffusion in the SBL is plume rise. The final rise is shown by Briggs (1975) to be

$$\Delta h = 2.6\left(\frac{F}{uN^2}\right)^{1/3} \tag{17}$$

where u and N are average values over the plume rise region. Agreement among theory, field data, and wind tunnel observations has been documented by Hewett *et al.* (1971). The buoyancy induced dispersion, σ_{z0}, at the final rise point is proportional to Δh and may substantially exceed growth due to the ambient turbulence; thus, it can determine the σ_z over a significant downwind distance (Weil, 1983). Since buoyant plumes are often near the top of or above the SBL, prediction of the SBL height may be most crucial to determining whether or not there is a ground-level impact.

2) Lateral diffusion

Lateral diffusion in the SBL is determined by the local turbulence, but it can be substantially accelerated due to wind direction shear. The latter is more pronounced in the SBL (than CBL) due to the weaker vertical momentum exchange with the consequent stronger Coriolis effects and to weak terrain slope influences. The overall σ_y can be shown to consist of two components expressed as (Csanady, 1969):

$$\sigma_y = (\sigma_{yt}^2 + 2K_e t)^{1/2} \tag{18}$$

where σ_{yt} is the turbulence induced dispersion. The latter can be represented by the same functional form used in the CBL [Eqs. (7) and (8)] and requires the measurement or estimation of σ_v and τ_{Ly}.

The K_e above is an effective diffusivity, which depends on the crosswind velocity distribution, boundary conditions, and time. For a constant crosswind gradient, dv/dz, and a $\sigma_z \propto t^{1/2}$, it has the following form at small times ($t \ll h^2/K_z$):

$$K_e = a(dv/dz)^2 K_z t^2, \tag{19}$$

where K_z is the vertical diffusivity ($=\sigma_w^2\tau_{Lz}$), which is assumed to be constant. The coefficient, a, varies with the boundary conditions, ranging from 0.018 for a surface source to 0.083 for an elevated release in an un-

bounded atmosphere (Smith, 1965). For a surface source in an Ekman layer, Csanady (1969) obtains the same expression (Eq. 19) with $a \sim 0.018$, but where dv/dz is given by the geostrophic wind divided by the Ekman layer depth. In the long time limit ($t \gg h^2/K_z$), the K_e tends to a constant (see Smith, 1965; Csanady, 1969).

c. *Applied models*

1) DIFFUSION

Applied diffusion models for the SBL have relied mostly on the K and statistical theories, with the latter receiving most use through the Gaussian plume model. In the following, we first cite examples where current SBL understanding has or could be used in improving the description of vertical dispersion. Then, we discuss lateral dispersion where a Gaussian profile should be adequate. In general, SBL models have not received as much attention as those for the CBL, due partially to the less complete knowledge of the SBL.

For surface sources, van Ulden (1978) developed a practical K model that showed good agreement with the numerical solutions of Nieuwstadt and van Ulden (1978), cited earlier, and the Prairie Grass data. The model predicts the ground-level concentration along the plume centerline to be

$$c = \frac{0.73Q}{2\pi\bar{u}\bar{z}\sigma_y} \exp[-(0.66z/\bar{z})^{1.5}] \qquad (20)$$

where Q is the source strength, $\bar{z}$ the mean plume height, and $\bar{u}$ the mean travel speed. The $x(\bar{z})$ and $\bar{u}(\bar{z})$ are expressed in terms of u_*, L, and z_0; the expressions are more complex than those in Gaussian models but reduction to simpler forms is possible.

For elevated sources in the surface layer, the Gaussian model and K theory can be used. However the K approach has two disadvantages in applications. First, the solutions for arbitrary $K(z)$ profiles can be more cumbersome to use than the Gaussian formula (see Csanady, 1973; Smith, 1957); this drawback might be alleviated by simpler parameterizations of them. Second and more serious, the approach is difficult to apply to a rising buoyant plume where plume "chunks" are brought to ground at close range. This problem is important in a high wind, weakly stable environment where the distance to final rise is large (Venkatram and Paine, 1984).

The Gaussian model can be used as a simple approximation in the surface layer provided that one chooses a suitable average wind speed and turbulence, i.e., pretends the layer is homogeneous. The wind speed is obtained from the similarity profile (Eq. 12 with the stable ψ function) by averaging over, say, $z_0 < z < 2h_s$; a suitable σ_w is an average value (Eq. 13) over the same range. The σ_z can then be estimated (Eq. 15) using these averages, assuming $t = x/u$, and choosing an appropriate τ_{Lz}. At short range, $\sigma_z = \sigma_w x/u$, which may be sufficient to estimate ground-level concentrations in the vicinity of the maximum.

The intent of the above is to introduce first-order effects of SBL structure into a Gaussian model for the surface layer. We regard this as estimating u and σ_z from the relevant parameters—u_*, L, and z_0, and believe that this has strong scientific merit and advantage over the more empirical Pasquill-Turner method. Moreover, some precedence exists, as Csanady *et al.* (1968) have applied the approach with success to field measurements in a neutral surface layer.

The most difficult sources to treat are those above the surface layer where one must seriously consider the z variation of σ_w as well as u. For simplicity, we consider the idealized SBL analyzed by Nieuwstadt (1984a) and a sufficiently large mixing parameter, γ, such that $\sigma_z \propto t^{1/2}$ at long times. There are three simple approaches that could be tried: 1) K theory with the K profile suggested by Nieuwstadt's model, 2) the Gaussian model with u, σ_w represented by average values and σ_z determined as above, and 3) the Gaussian model with a uniform wind but with the σ_w variation taken into account. The first and third options are most desirable because they explicitly address the σ_w and K inhomogeneities.

In general, there has been little testing of these simple techniques when dispersion takes place over a significant portion of the boundary layer. However, one example of the third option above is the model recently proposed by Venkatram and Paine (1984). They compute σ_z separately above and below the plume centerline, using a heuristic equation, based on the small time limit of statistical theory: $d\sigma_z/dt = \sigma_w(z)$. A comparison of their model with surface concentrations around tall stacks shows good performance and indeed much better than that attained with the CRSTER model.

For elevated sources and small mixing parameters $\gamma \sim 0.1$, the σ_z will level out ($\sigma_z \propto \sigma_w/N$) at least for some range of distances. The ground-level concentrations should then be zero or at least negligibly small. As pointed out earlier, the strong dependence of σ_z on γ emphasizes the need for more laboratory and field observations of dispersion as well as simple methods for estimating this parameter.

The estimation of σ_y from Eqs. (18) and (19) is best done using measurements of σ_v and dv/dz, which should of course correspond to the sampling time of the concentrations. The need for measurements is due to the lack of general and proven expressions relating σ_v and dv/dz to more readily available data. However, in high winds ($u > 7$ m s^{-1}), σ_v can be estimated from u_* through the surface layer relation $\sigma_v \sim 2.5u_*$. With a typical u_*/u (~ 0.04), the relation yields $\sigma_v/u \sim 0.1$, which is consistent with observations reported by Hanna (1983). In light winds, Hanna's observations suggest that σ_v becomes independent of wind speed and stability as do those reported by Pasquill (1974)

and others. The σ_v appears to be site dependent with values ranging from 0.3 to 1 m s^{-1}.

As in the CBL, the Lagrangian time scale (τ_{Ly}) is large and prediction of it is quite uncertain due to the presence (or not) of very large mesoscale eddies. Hanna's (1983) observations show that under light winds a typical τ_{Ly} is 120 min. whereas time scales from Briggs' empirical dispersion curves imply $u\tau_{Ly} = 5000$ m. For a 1 m s^{-1} wind, $\tau_{Ly} = 83$ min, in approximate agreement with Hanna's value, but for a 5 m s^{-1} wind, $\tau_{Ly} = 17$ min. Clearly, much more modeling and analysis of field observations is necessary to better predict τ_{Ly}.

In principle, the crosswind shear can be predicted from drag law expressions coupled with surface layer measurements, but there is so much scatter in comparisons of predictions with observations (e.g., Melgarejo and Deardorff, 1974) as to question the utility of this approach. We reiterate that measurements are the best approach for obtaining dv/dz.

2) SBL VARIABLES

The diffusion models require measurements or estimates of a number of variables including: Q_0, u_*, h, $\partial\theta/\partial z$ (for N), $u(z)$, σ_w, σ_v, and dv/dz. Due to the lack of models to describe all SBLs, we would advocate measuring as many of these variables as possible—certainly σ_w, σ_v, dv/dz, and h; the h can be determined with an acoustic sounder (e.g., Caughey, 1982). In the event that σ_w is not measured at all or at the proper heights, it could be estimated from the first four variables above, assuming that the similarity profile (Eq. 13) applies. To make such estimates, we assume availability of wind and temperature measurements from a 10-m tower and cloud cover observations.

The heat flux can be found from knowledge of u_* and the turbulent temperature scale, θ_*, through $Q_0 = -\rho c_p u_* \theta_*$. Van Ulden and Holtslag (1983, 1985) give an expression relating θ_* to u_* applicable over a wide range of u_*. It is based on the surface energy budget and similarity profiles (for wind and temperature) and depends on several empirical, site-dependent parameters. For sufficiently large u_* (>0.1 m s^{-1}), a simple estimate of θ_* can be based on the total cloud cover (van Ulden and Holtslag, 1983; Venkatram, 1980b). For small u_* (i.e., very light winds), θ_* varies linearly with u_*. If wind and temperature are available at multiple heights, θ_* (and u_*) can be obtained by fitting observations to the similarity profiles (e.g., Nieuwstadt, 1978).

Given θ_* (or the θ_*, u_* relationship) and a reference wind speed, u_1, at some height z_1, the u_* can be found from the similarity profile (Eq. 12).

As shown by Holtslag (1984), the wind profile is adequately predicted over most of the SBL using the Monin-Obukhov expression, but with the dimensionless wind shear function proposed by Carson and Richards (1978). Holtslag found that this function performed well up to heights of ~200 m in the SBL during highly stable conditions. Van Ulden and Holtslag (1985) present a simpler empirical function that appears to perform just as well.

In principle, the turbulent boundary layer height, h, is best determined by a rate equation model such as Nieuwstadt and Tennekes (1981). However, that model depends strongly on the initial estimate of h at evening transition, for which there is no model. A number of authors (Arya, 1981; Mahrt *et al.*, 1982; Nieuwstadt, 1984b; Venkatram, 1980b) have suggested and shown that rough estimates of h can be given by Zilitinkevich's (1972) steady state expression: $h = b(u_* L/f)^{1/2}$ where b ranges from 0.4 to 0.7. Thus, while perhaps inferior in principle, this expression appears to work.

The thermal boundary layer height, h_T, generally exceeds the height of the turbulent layer, due to radiative cooling. The h_T and potential temperature profile, $\theta(z)$, can be predicted from a heat flux integral model such as Stull's (1983), at least during light wind (~2 m s^{-1}), strongly stable conditions (see discussion by van Ulden and Holtslag, 1985). The model defines a length scale for the temperature profile in terms of the integrated heat flux and the surface temperature change (with time). The assumed temperature profile is of a similarity form and is found to agree well with data from the Wangara and Koorin experiments. For higher winds (~10 m s^{-1}) in which a deeper turbulent layer exists, van Ulden and Holtslag (1985) show that a "triple structure" temperature profile exists. They indicate that Wetzel's (1982) model may be more suitable in approximating this structure, but it requires the wind speed at the SBL top; this wind is usually not available. Thus, a simple method for adapting Wetzel's model or modifying Stull's is needed to describe the temperature profile over a broad range of wind speeds.

d. Recommendations

Our review has indicated much recent progress toward understanding the SBL: its structure, diffusion within it, and the parameterization of controlling variables. But on balance, we view this understanding as incomplete and feel that we cannot now recommend placing models based on new knowledge into general practice. There were indeed differing views on this point expressed at the workshop, with some participants favoring immediate adoption of new techniques by regulatory models. However, the consensus was that more development and testing of such techniques were necessary before putting them into widespread use. This position should not be taken as an endorsement of current practice; its deficiencies are fully recognized as stated in the Introduction. With these remarks in mind, the following suggestions are made:

1) *SBL structure*—A program is recommended to develop general engineering models for SBL structure

and the variables (u_*, Q_0, h, etc.) controlling it. This should be done at a number of sites representing different real world conditions, e.g., flat and rolling terrain with varying roughness. The program would include a number of steps: (i) assembling existing data bases on vertical structure of u, θ, σ_w, σ_v, heat flux, etc. and possibly gathering new ones, (ii) comparing observed structure to predictions from turbulence closure and rate equations, (iii) investigating the SBL horizontal structure, primarily from observations, and (iv) developing engineering correlations for the structure for use in applied diffusion models.

2) *Applied diffusion models*—Our principal recommendation is to test the applied models discussed under section 3c1 or others with existing data bases or new ones. For example, with sources above the surface layer the approaches could include: K theory using Nieuwstadt's (1984a) K profile and the Gaussian model with layer averaged u, σ_w or average u but a $\sigma_w(z)$ profile. The main point is to test models that explicitly incorporate those SBL variables (u_*, Q_0, h, etc.) controlling turbulence, mean wind, etc. It is felt that a reanalysis of datasets such as those used by Irwin (1983) would be of great value in determining how well these schemes work. One of the main challenges will be the determination of the key SBL variables from very rudimentary observations in earlier experiments.

3) *SBL variables*—It is recommended that the methods for estimating u_*, Q_0, h, h_T, etc. discussed under section 3c2, or alternatives, be evaluated with many more datasets, and especially those covering a variety of surface conditions. Note that the methods discussed here have in general only been tested at one or a few sites.

4) *Data bases*—The development and testing of models may be severely limited by existing data bases; more complete ones are necessary. However, they should include numerical and laboratory simulations (wind tunnels, water channels) as well as field data. We especially urge that simulations be pursued to provide fundamental information for the development of applied models; the CBL is a good example where such simulations have been of much benefit. For example, the continuous flow water channel of Stillenger *et al.* (1983) can simulate strongly stable stratification and may be a good facility for exploring fundamental questions concerning the mixing parameter γ and the σ_z versus t behavior. Second-order closure models have already been used to explore SBL structure over ideal flat terrain (Brost and Wyngaard, 1978), but could be used for other terrain types and be linked to a diffusion model.

5) *Key problems*—With regard to SBL structure, the main problems and uncertainties relate to nonideal terrain, nonstationarity, waves, intermittency and local drainage. Others include a model for the SBL height, h, at evening transition and general, workable methods for estimating σ_v, dv/dz and τ_{Ly} in lieu of direct observations. With respect to diffusion, the problems are the σ_z behavior at long times, simple methods for estimating γ, and the treatment of diffusion when it occurs over a significant depth of the SBL. To this list, we should add diffusion under light winds where a puff model approach should be considered.

4. Model uncertainty

The previously discussed models predict the mean or ensemble-averaged concentration for a given set of source and meteorological conditions. As is well known, the comparison of predictions to observations, taken under supposedly the same conditions, will reveal large deviations between the two (deviations ~ mean). The deviations have a mean or bias and a variance. The bias is due solely to internal model errors (e.g., physics, parameterizations, etc.), whereas the variance is due to four factors: 1) uncertainty in model input variables, 2) errors in the concentration measurements, 3) internal model errors, and 4) natural or inherent variability (see Fox, 1984, Venkatram, 1982).

All of the above factors can contribute significantly to the variance with the first two varying with the quality and (space or time) resolution of the measurements or inputs. However, it was the intent of this workshop to only focus on the natural variability, which is typically a major component of the variance. Formally, the natural variability can be defined as

$$\sigma_c = \langle (\bar{c} - \langle \bar{c} \rangle)^2 \rangle^{1/2} \tag{21}$$

where the overbar denotes a time average and the angle brackets indicate an ensemble average. In the following, the omission of an overbar designates an instantaneous concentration and a prime denotes a deviation about the ensemble mean. In stationary turbulence, $\langle c \rangle = \langle \bar{c} \rangle$.

Natural variability arises because the details of the initial and boundary conditions describing the flow are not the same in individual realizations, even though the gross conditions (e.g., mean wind speed, heat flux) defining the ensemble are. As discussed under section 4c, the natural variability is dependent on the ensemble, varying with the choice and number of conditions defining it. When the natural variability is large ($\sigma_c \sim \langle \bar{c} \rangle$), the mean concentration alone is inadequate to predict the range and probability of concentration levels. It must be supplemented by an estimate or model for σ_c as well as the functional form of the $\bar{c}$ pdf (some models also require the intermittency). Such information is necessary in predicting the expected exceedances of specified concentration levels (standards) and in the evaluation of models for the mean concentration. To date, natural variability estimates have essentially played no role in assessing the attainment of standards; however, they should and hopefully will in the future.

In the following, we briefly review the physics of concentration fluctuations, models for predicting nat-

ural variability and their role in mean model evaluation, and our recommendations. We use the terms concentration fluctuations and natural variability interchangeably.

a. Physics of concentration fluctuations

To visualize the processes that cause concentration fluctuations, we consider a small gradually expanding instantaneous plume that is bodily distorted by large scale eddies. There are two primary sources of fluctuations. First, the instantaneous plume entrains uncontaminated ambient air due to eddies comparable in size or smaller than itself. This process leads to an inhomogeneous profile across the plume and to fluctuations over scales smaller than the plume width. Laboratory experiments (Fackrell and Robins, 1982; Netterville, 1979) and some field observations (Hinds, 1969) show that the relative intensity of fluctuations, $i_p = (\langle c'^2 \rangle / \langle c \rangle)^{1/2}$, typically ranges from 0.5 to 1.5 for conditional samples that exclude zero concentrations. Such samples and the intensity based on them are somewhat ill-defined, in general, because they depend on instrument resolution, i.e., how a "zero" concentration is defined.

The second source of fluctuations—meandering—can cause even larger fluctuation levels at a fixed receptor as the latter is alternately exposed to different parts of the plume. More importantly, meandering can cause the concentration to vary essentially between "in-plume" peaks and the zero ambient value. Thus, it can lead to total fluctuation intensities, based on zero and nonzero concentrations, much greater than 2 and depending, in general, on source size, height, and buoyancy. Meandering is an important source of fluctuations as long as the plume dimension is smaller than the energy containing eddy scale (i.e., $t < \tau_L$). (For meandering or intermittent plumes, the total fluctuation intensity depends on i_p and the fraction of the time of nonzero concentrations; see Wilson *et al.*, 1985.)

In the CBL, vertical meandering is an important source of concentration variance for an elevated source because of the large eddy size ($\sim z_i$) and the long time scale ($\sim$ 10 min). Lateral meandering is important in both the SBL and CBL because of the long (but ill-defined) time scale of the lateral turbulence.

The above picture of concentration fluctuations has emerged from modeling, field observations, and laboratory experiments. Toward that end, laboratory experiments have been very beneficial. For example, the Fackrell and Robins (1982) experiments, conducted in a neutral wind tunnel flow, clearly show that the fluctuation intensity, at the ground, is much greater for an elevated than a surface source, due to the greater role of meandering. The experiments also demonstrate that source size is important for the elevated release whereas it is not for the surface source. In addition to these experiments, those of Deardorff and Willis (1984) have simulated many interesting features of the variance field in the CBL; for example, the fluctuation intensity at the surface is greater for a buoyant than a nonbuoyant release, due presumably to the more elevated plume axis.

b. Models for concentration fluctuations

There is a need for simple applied models as well as more numerically detailed, research models to address concentration fluctuations or natural variability. The applied models are the real working tools for mean model evaluation and air quality assessment. The research models are necessary for obtaining new insights and for providing "test" data for the applied models.

1) APPLIED MODELS

Essentially two types of applied models have been developed for concentration fluctuations: the meandering plume (Gifford, 1959) and the Eulerian similarity model (Csanady, 1967). Several variants of each have been formulated. The meandering model describes the fluctuations due to the large scale eddies alone and is appropriate when the latter scale exceeds the "instantaneous" plume dimension. In contrast, the similarity models treat the fluctuations due to "in-plume" turbulence alone. Since Csanady's and most other models have their origin in K theory, they are strictly legitimate only when the plume width exceeds the characteristic eddy scale (i.e., $t > \tau_L$).

In Gifford's model, the instantaneous plume is assumed to be nonrandom and Gaussian. By assuming the plume meander statistics to also be Gaussian, Gifford derived an expression for the ensemble variance ($\langle c'^2 \rangle$) field to be:

$$\langle c'^2 \rangle = \left(\frac{Q}{2\pi u \sigma_i} \right)^2 \frac{1}{(2\sigma_m^2 + \sigma_i^2)} \times \exp\left(- \frac{y^2 + z^2}{2\sigma_m^2 + \sigma_i^2} \right) - \langle c \rangle^2 \quad (22)$$

where σ_i and σ_m are the standard deviations of the instantaneous plume and meander, respectively. (Here, the standard deviations are assumed to be equal in the y and z directions.) The meandering model is supported by the Fackrell and Robins wind tunnel experiments for an elevated source. For example, the experiments show an approximate Gaussian form in z for the variance field and a power law pdf for c' on the elevated plume centerline.

In a similar but simpler analysis, Venkatram (1979) considered the ground-level concentration time series due to a meandering plume to be either a maximum, c_{max}, when the plume is over a receptor or zero when it is not. The ensemble variance is then $\langle c \rangle^2 (\Gamma - 1)$, where Γ is the peak-to-mean ratio, $c_{max}/\langle c \rangle$. The c_{max} and $\langle c \rangle$ can be estimated based on the growth of the

instantaneous and ensemble-averaged plumes: different expressions are necessary for the instantaneous plume growth depending on whether it is passive or buoyant.

In most applications, one needs to know the variance in concentrations averaged over some time T_a, say one-hour (as indicated by the overbar). Provided that the autocorrelation function, $R(t)$, for the concentration time series is known, the variance in the one-hour means can be estimated from

$$\langle(\bar{c} - \langle c\rangle)^2\rangle = \frac{2\langle c'^2\rangle}{T_a}\int_0^{T_a}\left(1 - \frac{t}{T_a}\right)R(t)dt \quad (23)$$

(Lumley and Panofsky, 1964); here, the turbulence is assumed to be stationary, i.e., $\langle\bar{c}\rangle = \langle c\rangle$. Sykes (1984) has given a simple means of applying Eq. (23) in which the integral time scale of the concentration is estimated from the integral scale of the velocity fluctuations. His result, as well as Venkatram's (1979), show that the variance is proportional to $\langle c\rangle^2$. This finding appears consistent with observations of ground-level concentrations around tall stacks during convective conditions. (It should be remarked that in general a major problem in applying Eq. (23) is the nonstationarity of the atmosphere and knowledge of the integral scale, particularly for the lateral turbulence component.)

In an approach related to the meandering plume, Venkatram (1984) extended the pdf model for the mean concentration field (section 2c1) to that for estimating the variance in time-averaged samples. The main hypothesis is that the variance is caused by the unknown variation of the pdf's of vertical and lateral velocity fluctuations over the sampling period. Venkatram's expression for the ground-level concentration variance is applicable to an elevated source in the CBL.

In contrast to the statistical nature of the meandering model, the basis of the Eulerian similarity models is Csanady's (1967) differential equation for the concentration variance. In addition to adopting K theory, Csanady assumed self-similarity of the mean and variance fields in order to obtain simple solutions to the variance equation. Csanady (1973) showed that the model described data from some laboratory experiments and a lake dye study, but the value of an adjustable parameter varied in an unknown manner between the experiments.

A variety of simplifications and adaptations of the basic model have been made (e.g., Netterville, 1979; Hanna, 1984; Wilson *et al.*, 1982a,b). The simplest yields a Gaussian distribution for the variance. In most models, the σ_y and σ_z of the variance field are the same ones used for the mean concentration field. The source strength is the hypothetical "source variance intensity" ($\langle c'^2\rangle/\langle c\rangle^2$) that would have to be released at the stack in order to match the downwind variance profiles. It is an artifact necessary to bridge the near field, where variance production due to meandering dominates, and the far field where the similarity model applies.

Several empirical expressions based on wind tunnel experiments have been developed for the functional form of the source intensity. There is some agreement that it depends on the ratio of the turbulence integral scale to the source size, with the ratio raised to some power between ½ and 1.

When plumes diffuse near or toward the ground, an "image" sink is introduced to account for the increased dissipation of variance near the surface (Netterville, 1979). The height of the "effective variance source" and the strength of the image sink are variables in general and can be fitted to observations. Wilson *et al.* (1982a) have used Fackrell and Robins (1982) wind tunnel data for this purpose and found that a ratio of sink strength to "real" source strength of 0.6 is necessary for a near surface release. For an elevated release, Wilson *et al.* (1982b) found that the variance field far above ground is not very sensitive to the surface boundary condition. Thus, it is difficult to evaluate the utility of any models for predicting concentration variance at the surface on the basis of their performance above ground.

Of the two general approaches discussed here, the meandering model would seem to have the most immediate application to the large concentration variances associated with an elevated source in the CBL, at least in the "near source" region. This is due to the long time scale of the large eddies. The meandering model may apply over an even more extensive downwind range because of the long time scale of the lateral velocity fluctuations; this is true for the SBL as well as the CBL. An important problem with both model types is the extension and inclusion of plume buoyancy effects into the variance predictions. For the similarity models, a worthwhile development effort is a more direct analytical linkage of the source intensity variance in the far field to the variance production in the near field—the meandering phase.

2) RESEARCH MODELS

Three types of research models have received much attention recently: Lagrangian, second-order closure, and "core–bulk." Lagrangian models (Durbin, 1980; Lamb, 1980; Sawford, 1983) are based on the two-particle pdf; i.e., the pdf of simultaneously observing particle 1 at x_1 and particle 2 at x_2. The pdf is generated by a stochastic model, which predicts separation and center-of-mass variables for particle pairs in a specified flow field. To date, such models have considered dispersion in one dimension and have been solved by Monte Carlo or other techniques.

Application of the Lagrangian model to a small source in neutral, homogeneous turbulence (Durbin, 1980; Sawford, 1983) shows a number of interesting and promising features. One is that the concentration fluctuation intensity depends on the ratio of the source size to the turbulence integral scale. This result is a consequence of inertial range scaling and is supported

by the Fackrell and Robins (1982) data discussed earlier.

Thus far, the Lagrangian models have been used to study idealized sources in highly idealized flows—neutrally stratified, homogeneous turbulence. However, the approach could be applied in principle to other more realistic flows, the CBL and SBL, when coupled to the appropriate velocity field. For example, the CBL flow has been generated by a large-eddy simulation model (Deardorff, 1972) and the SBL field by a second-order closure model (Brost and Wyngaard, 1978). We see the coupling of the Lagrangian models and the above flow fields to be of great potential utility in generating the c' statistics for testing and developing the applied models. This is also discussed by Wyngaard *et al.* (1984).

The second-order closure model is based on a differential equation for concentration variance (as in Csanady, 1967), which itself is part of a large set of coupled, partial differential equations for mean, flux, and second moment quantities. Like the Lagrangian models, it is most useful as an investigative tool to examine fundamental issues including complex and realistic flows. Sykes *et al.* (1984) applied a second-order model to the prediction of concentration fluctuations in a neutrally stratified flow. Upon adjustment of a few parameters, their model matched the wind tunnel results of Fackrell and Robins quite well, including the source size effects. Their model is constructed in such a way as to simulate the initial meander phase as well as the long time behavior, for both the mean and variance fields.

As with the Lagrangian models, the calculation of concentration fluctuations with the second-order approach should be linked to more realistic flow fields. Such models have already been applied to the simulation of the mean flow and turbulence in the CBL and SBL; they may be more suitable for the latter (e.g., Brost and Wyngaard, 1978). In addition to this extension, the approach needs modification to incorporate plume buoyancy effects.

The core–bulk model (Chatwin and Sullivan, 1979) is applicable only to relative dispersion and has been developed mostly for clouds. It predicts the cloud to have a small core region, in which the mean and concentration variance are large, surrounded by the bulk of the cloud in which $\langle c \rangle$ and $\langle c'^2 \rangle$ are much smaller. In a number of flows, a self-similar structure of the mean concentration and variance evolves, but as with the Lagrangian and second-order models, the initial cloud dimension is "remembered." This model would have to be extended to include meandering effects in order to be useful in generating c' statistics for applied model development.

c. *Role of natural variability estimates in mean model evaluation*

An effective method of evaluating models for the mean concentration is to analyze the statistics of the deviation between predictions ($\bar{c}_{\text{pred}}$) and observations ($\bar{c}_0$), i.e., the residual d:

$$d = \bar{c}_0 - \bar{c}_{\text{pred}},$$

(Electric Power Research Institute, 1978; Fox, 1981; Venkatram, 1982). Ideally, the residuals should be uncorrelated with the model inputs and the output; i.e., they should have a zero mean and a variance independent of the input variables. There are two issues of concern here: 1) the choice of an ensemble of observations, and 2) the use of natural variability estimates in the residual analysis.

In classical treatments of turbulence, an ensemble is defined in terms of the fixed external conditions and a well-defined turbulence time scale; e.g., as in a wind tunnel experiment. However, in the atmosphere, the time scale for the lateral turbulence is not well defined in either the CBL or SBL; thus, the constancy of τ_L cannot be guaranteed. In addition, field experiments cannot be conducted under fixed conditions for arbitrarily long sampling times because conditions change. Moreover, for pragmatic reasons, the list of fixed conditions will not contain all variables that will affect the concentrations (e.g., skewness and higher moments of the turbulence velocity field). Therefore, one approach in model evaluation is to define an ensemble in terms of the model inputs, which are determined for a specified averaging time (Venkatram, 1982).

In general, the observed concentration or sample mean can be expressed as

$$\bar{c}_0 = \bar{c}_0(\xi, \eta), \tag{25}$$

where ξ represents the model inputs and η refers to variables that are not measured or known in an experiment (and may indeed vary from realization to realization). Equation (25) can be rewritten as

$$\bar{c}_0(\xi, \eta) = \langle \bar{c}_0(\xi, \eta) \rangle + \bar{c}'_0(\xi, \eta) \tag{26}$$

where the averaging is over all realizations with ξ held fixed.

The variance, $\langle \bar{c}'^2_0 \rangle$, at a fixed ξ is important because it is a major component of the residual variance, $\langle d^2 \rangle$. In the case of zero measurement errors and no uncertainty in the input variables, the latter is given by Fox (1984) as:

$$\langle d^2 \rangle = \langle d \rangle^2 + \langle \bar{c}'^2_0(\xi, \eta) \rangle \tag{27}$$

where $\langle d \rangle$ is the bias or mean residual at a given ξ. From the above, it can be seen that if $\langle \bar{c}'^2_0 \rangle$ varies with ξ, $\langle d^2 \rangle$ will also; thus, one cannot construct a residual plot independent of model inputs. (A good example is the dependence of the concentration variance on distance for an elevated source.)

There are two ways of determining the variance, $\langle \bar{c}'^2_0 \rangle$. First, if ξ contains n variables, one can "bin" observations into small volumes in n-dimensional space and determine the rms deviation, $\sigma_c(\xi)$, for each. The disadvantage is that it requires an inordinate

number of observations under the "same" conditions, a difficult task in practice. The second approach (Venkatram, 1982) is to assume that the shape of the $\bar{c}'_0(\xi, \eta)$ pdf is independent of the model inputs (ξ) and that $\bar{c}'_0(\xi, \eta)$ can be represented as $\bar{c}'_0(\xi, \eta) = \mu(\eta)\sigma_c(\xi)$, where $\mu(\eta)$ is a random variable. The pdf of μ represents a "shape factor" which is to be determined empirically. The variance, $\langle \bar{c}'^2_0 \rangle$, is then $\sigma_\mu^2 \sigma_c^2$ where σ_μ^2 is the variance of μ. Use of the latter in Eq. (27) results in:

$$\frac{\langle d^2 \rangle}{\sigma_c^2} = \frac{\langle d \rangle^2}{\sigma_c^2} + \sigma_\mu^2, \tag{28}$$

where one has normalized out the known variation of σ_c. Equation (28) indicates that a plot of d/σ_c is independent of model inputs provided that $\langle d \rangle/\sigma_c$ is acceptably small.

Application of Eq. (28) requires a model for concentration fluctuations, $\sigma_c(\xi)$, as well as for the mean concentration. The σ_c models are those discussed previously under 4.B. Admittedly, some iteration of the mean and fluctuation models may be necessary to indeed achieve a plot of d/σ_c that is independent of model inputs.

d. Recommendations

Our review has indicated the need to incorporate natural variability estimates into concentration prediction schemes and into residual analyses of mean models. We have identified simple models of two general forms, meandering and Eulerian similarity, that may be suitable for use. However, at present, there is little feel for how these models will perform in actual applications due to their sparse testing with field data or with laboratory simulations (of the CBL or SBL). Therefore, we cannot recommend a scheme to implement now. Instead, it is recommended that the models discussed be tested and developed as necessary according to the following suggestions. We reiterate that natural variability estimates are a logical part of the air quality prediction process and that they can and should ultimately become part of it.

1) *Applied models*—Our main recommendation is to test, develop, and generally gain experience with the models discussed, using measurements from real or simulated boundary layer experiments. At present, the CBL offers the best opportunity to do this because of the good or better standing of mean models and because of the existence of field and laboratory data. The meandering model or variants of it have the most applicability for the near source, large σ_c regions due to the large eddies and time scales involved. We urge the analysis of field, laboratory, and (future, hopefully) numerical data with them. However, in applying the meandering model per se to time-averaged concentrations, one needs an estimate of the concentration integral time scale (see Sykes, 1984).

2) *Evaluation of mean models*—The analysis of residuals is an effective method of evaluating mean concentration models, but this must be done in light of the concentration fluctuations. To attain a residual plot that is independent of model inputs, it is recommended that the residuals be normalized by the rms concentration fluctuation, σ_c. Several iterations of this approach may be necessary to assess its merits as it has not generally been practiced.

3) *Data bases*—It is recommended that the applied models be evaluated with all relevant data and, in particular, that further laboratory and numerical simulations be conducted for this purpose, with emphasis on the CBL. Additional experiments in the Willis and Deardorff convection tank should span a broad range of buoyancy fluxes: $F_* < 0.05$ where the plume remains well within the CBL and has a highly fluctuating axis, as well as larger F_*, where the plume rises mostly to the CBL top before diffusing downward. We recommend that the research models, Lagrangian statistical and second-order closure, be linked to more realistic flow field simulations (e.g., large-eddy simulation of the CBL) and that one generates concentration fluctuation statistics for a range of stack heights and buoyancy fluxes. It is recognized that further development of these models is necessary to accomplish this. In addition, it must be remembered that neither these models nor the laboratory counterpart will simulate all the variance associated with large mesoscale eddies.

4) *Key problems*—Our review has found that the following are key problems to pursue: i) the prediction of the concentration fluctuations due to source buoyancy, ii) the general functional form for the σ_c dependence on source size, and iii) knowledge of the time scale of the large mesoscale eddies. The last is particularly important in determining the range of applicability of the meandering model. We should add that there is a general lack of observations and information on concentration fluctuations in the SBL and that models and experiments are needed to fill this void.

5. Summary

For some time, a wide gap has existed between diffusion modeling "science" as it is generally practiced in the regulatory community and as it is understood in the framework of PBL structure. The Clearwater workshop was organized to help close that gap. Specific workshop purposes were to review current understanding of PBL structure and diffusion and to recommend how it could be used to improve applied models—their physics and hopefully their performance. Three main areas were addressed: diffusion in the CBL, diffusion in the SBL, and model uncertainty.

Progress has been made in all areas, but it is most significant and ripe for application in the case of the CBL. This stems from a well-documented picture of the CBL's mean and turbulence structure, the latter

being predicted largely on the basis of convective scaling (w_*, z_i). In addition, investigations of tracer diffusion in the laboratory, field, and with numerical simulations have shown salient features. Furthermore, some of this knowledge has already been put to use in applied models and shows much promise.

Based on our CBL review, a number of recommendations have been made on the use of new knowledge in applied modeling (section 2d). For the short term, a Gaussian model is recommended, but for the long term, the pdf and impingement models should be considered. Perhaps our strongest recommendation is on the use of convective scaling in estimating dispersion parameters (σ_y, σ_z); here, clear success has been demonstrated with field, laboratory, and numerical data. Some general σ_y, σ_z expressions are discussed for arbitrary stability, where the latter is characterized by $z_i/-L$ or u/w_*. Additionally, methods for estimating key CBL variables—u_*, Q_0, u, z_i—are recommended. Further details and important technical problems are given in Section 2.

By comparison to the CBL, our understanding of turbulence structure and diffusion in the SBL is less complete, but there have been recent promising developments. For example, a similarity framework now exists for predicting the structure over ideal, flat terrain, and it has been successfully tested. However, the complications arising from nonstationarity, local drainage, and waves, which are typical of "real" sites, must be addressed. For elevated source diffusion, models have been advanced to predict σ_z in terms of the local structure. But there is a controversy on the behavior of σ_z at long times, and further field, laboratory, and numerical data are necessary to address it.

As a result of our SBL review, we cannot now recommend adoption of these recent developments by applied models due to some of the uncertainties raised. Instead, a development program is recommended (section 3d). For SBL structure, it is suggested that the similarity framework be tested with existing and new data sets from a variety of sites representing different conditions. From this effort, useful engineering models for structure would be developed. For diffusion, it is recommended that simple models, based on K theory or the Gaussian plume (section 3c), be tested and developed with existing and new data. Methods for estimating key SBL variables were identified, but they also require further evaluation. Of crucial importance to this development effort is the generation of new data sets. In this regard, we strongly urge that numerical and laboratory simulations be pursued as a useful complement to field observations.

For model uncertainty, we recognize and urge that natural variability estimates become an integral part of air quality predictions. Such estimates are also needed in the evaluation of models for the mean concentration. We have identified simple models of two general forms—the meandering plume and Eulerian similarity—that would be suitable for use. However, there is little experience with the performance of such models in applications; therefore, we do not recommend implementing a scheme now.

As with the SBL, it is recommended that the models be tested and developed as necessary using all relevant field, laboratory, and numerical data. This should be tried first for the CBL because of our better understanding of it and the availability of some observations. Again, a major requirement is the generation of data sets. Because of the expense of field observations, our view is that laboratory and numerical simulations should play a key role The convection tank facility discussed in Sections 2 and 4 should be ideal for the CBL and be pursued further. Numerical simulations would be useful in generating concentration fluctuation statistics for a variety of source heights and buoyancy fluxes. Here, we envision the coupling of a Lagrangian statistical or second-order closure model to realistic flow field simulations (e.g., large-eddy simulation of the CBL).

As should be apparent from our review, the key to building better applied models is understanding the mean and turbulence structure of the PBL. In this regard, a close association of the applied modeling and research communities is required. Some improvement along these lines has occurred over the past 5–10 years as demonstrated in part by the mix of participants in this workshop. However, a significant part of the applied modeling community is unaware of the developments in PBL research. This needs improvement perhaps by short courses and by strengthening the AMS symposium on applications.

Our review has identified a number of technical problems needing resolution. To keep track of them, it may be useful for the AMS Steering Committee for the EPA Cooperative Agreement to review the status of models every 3 years or so and to revise the list of problems and priorities. By models, we mean those for the relatively ideal problem considered here—an elevated point source in essentially flat terrain. For if this cannot be properly addressed, how can one consider the complications arising from complex terrain, plume chemistry, etc.?

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